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HPTLC-ESI-MS/MS for identifying neutral lipids, sphingolipids and phospholipids in complex samples

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HPTLC is well-adapted to providing lipid-class separations, as an assistant technique of HPLC. From this perspective, it can complement traditional LC-mass spectrometric approaches in a unique way. As the zones of interest on the plate can selectively be transferred to the ESI-MS instrument via an elution head-based interface, a rapid, relevant structural information about molecular species within each lipid classes from complex samples can be obtained.

Separation using AMD2 provides lipid-classes as narrow peaks enough to ensure a direct elution and transfer of the plate zones to obtain both composition profiles of each class by ESI-MS, and identification of individual lipids and molecular species belonging to each separated lipid class by MS/MS (MS^n) and HRMS. The respective sodium adducts of the above-mentioned lipid classes were fragmented in the positive ion mode using an ion-trap technology. The sodium remained the charge of their fragment ions, thus being useful for their structural identification by MS/MS (MS^n) through further fragmentation.

This work exemplarily focuses on profiling and identification of neutral lipids (NLs), sphingolipids (SLs) and phospholipids (PLs) in three analytical cases:

(1) mono- (MAGs) and diacylglycerides (DAGs) in positive ion mode and fatty acids (FAs) in negative ion mode as impurities in a fatty acid methyl ester-based biodiesel

(2) molecular species of neutral sphingolipids (SL), such as sphingomyelins (SMs) and globotriaosylceramides (Gb3), in human plasma

(3) phosphatidylcholines (PCs), phosphatidylethanolamines (PEs), phosphatidylglycerols (PGs) and cardiolipines (CLs) associated to membrane proteins of photosynthetic purple bacteria.